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Application of a Random Choice Method to Small Amplitude 2D Shockwaves

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Abstract

Sampling techniques and exact solutions of Riemann Problems are used in a random choice method. This procedure is used to obtain the numerical solutions of a system of conservation laws which describes the dynamics of flow for small amplitude two-dimensional shockwaves. An intrinsic coordinate system is used to formulate the model.

1 Introduction

Accuracy of numerical solutions and efficiency of numerical schemes are major concerns in obtaining numerical solutions. Moreover, the numerical solution at the jump discontinuities called shocks should remain sharp, stable and transports the discontinuities at the correct physical speed. Random variables have been used to control numerical dissipation or to control numerical viscosity. Basically, random variables appear either as a component added to the deterministic equation to study the effect of numerical viscosity or they are used to sample the solution at a randomly chosen point to obtain a numerical solution which preserves some mathematical properties of the solution function. The purpose of this paper is to present a random choice method for computing the numerical solution of two-dimensional small amplitude shockwaves. The numerical random sampling procedure is a shock capturing and a marching time method for solving system of conservation laws. The random sampling procedure consists of approximating the numerical solution by a piecewise constant state at each time step and proceeding to the next time step by solving the corresponding problems formed by the constant on the neighboring spatial intervals. It is well-known that the exact solution of non-linear system of partial differential equations arising in fluid flow problems even with smooth initial data develops shocks (jump discontinuities) in a finite time interval. Thus it is not unnatural to approximate their initial data with constant states.

The sampling procedure is based on approximating the numerical solution of the given problem with a sequence of elementary problems, known as the Riemann problems. These Riemann problems can be thought of as information source about the solution within each spatial mesh interval. More importantly they provide valuable information on wave interaction.

Godunov [1] initiated utilizing the solutions of the Riemann problems as building blocks for the construction of numerical solution of the nonlinear hyperbolic partial differential equations. Godunov replaced the initial data by a piecewise constant states with jump discontinuities at the middle of spatial mesh interval. Then the exact solution of this Riemann problem at the first time step is calculated. To proceed to the next time step replace this exact solution by a new piecewise constant state approximation and solve the corresponding Riemann problem and maintain integral properties of the conserve variable.

Another utilization of Riemann problems in obtaining the solution of conservation laws was initiated by Glimm [2] who followed Godunov as far as obtaining the exact solution of Riemann problem and then the value of the new approximated solution at the new time step is taken to be the exact solution evaluated at a random point on that mesh interval. This solution is conservative on the average, however, has the advantage that near jump the solution is incremented either by the amount of jump or not at all. This forces that an initially sharp discontinuities remains sharp. Chorin [3] developed Glimm's random choice method into a numerical technique. The random choice method by its way of construction propagates shocks without introducing any dissipation and the method is unconditionally stable. However, because of approximating solution at a randomly chosen point a small amount of statistical noise enters into the solution which is acceptable within the accuracy imposed by discretization of model problem.

2 Two-Dimensional Flow Problem

The equations describing the two-dimensional flow of shockwaves with a source term in fluid dynamics for compressible fluid may be written in the form

$$(1) \qquad u_t + f(u)_x + g(u)_y = h(u, x, y, t)$$

where f and g are physical fluxes, h is a source term and the unknown quantity, u is a function of x, y, t. Denoting the front coordinate by α and letting the coordinate β be

the arc length measured from a reference point along the front, then the successive front positions are given by the family of curves, α = constant and the ray positions by the family of curves, β = constant. By using this intrinsic coordinate system α β (see Whitham [8]) where α and β are functions of x, y, t, equation (1) can be written as

$$w_\alpha + F(w)_\beta = G(w, \alpha, \beta) \tag{2}$$

subject to the initial condition given by

$$w(0, \beta) = w_0(\beta) . \tag{3}$$

Equations relating x and y to α and β are given by

$$x_\alpha = (1 + \tfrac{1}{2} m\phi)\cos(\theta) \quad x_\beta = -A\sin(\theta)$$

$$y_\alpha = (1 + \tfrac{1}{2} m\phi)\sin(\theta) \quad y_\beta = A\cos(\theta)$$

Here θ is the angle that each front makes with the positive x-axis, A is the cross-sectional ray-tube area, and m is the acoustic Mach number. For small amplitude two-dimensional shockwaves we have

$$w = \begin{pmatrix} A \\ A\theta \\ m\sqrt{A} \end{pmatrix} \qquad F(w) = \begin{pmatrix} -\theta \\ (m\phi - \theta^2)/2 \\ 0 \end{pmatrix},$$

$$G(w) = \begin{pmatrix} 0 \\ 0 \\ -\dfrac{\phi A m^3}{4CZ} \end{pmatrix} \tag{4}$$

where C is the local sound speed, ϕ is the nonlinearity constant which depends on the media and Z is the area under the initial pulse. For a detail discussion of these equations see Zakeri [4]-[5]. To solve (2)-(3) we use operator splitting method to remove the inhomogeneous term G(w, α, β). That is, first we solve the corresponding one-dimensional homogenous problem,

$$w_\alpha + F(w)_\beta = 0 \tag{5}$$

by sampling procedure and then we use its solution to determine the value of the inhomogeneous term, G(w, α, β). Finally, we solve the corresponding ordinary differential equations (ODEs) given by

$$w_\alpha = G(w, \alpha, \beta) . \tag{6}$$

To solve (6) we use a common ODE solver such as Runge-Kutta or a multi-level method.

3 Numerical Scheme

We develop a numerical scheme to compute the successive shock fronts using geometrical shock dynamics given by (2)-(3). One of the advantages of formulation of a model problem using geometric shock dynamics is its simplicity. To develop a random choice method first we must define a random variable defined over closed interval [-½, ½]. It is absolutely necessary that the successive values of the random variable tend to approximate equi-partitioning the closed interval [-½, ½] (see Glimm [2]). To generate such random variable let us consider a sequence of pseudorandom integers generated by

$$N_{n+1} = N_n + \left[\frac{3-\sqrt{3}}{6} k\right] \quad (\mathrm{mod}\ k) \tag{7}$$

where k is an odd positive integer and N_0 is an arbitrary integer less than k. Let us define an equidistributed sequence random variables, σ_n on the interval [-½ , ½] given by

$$\sigma_n = \frac{N_n}{k} - \frac{1}{2} . \tag{8}$$

We introduce front-ray grid defined by mesh lengths $\Delta\alpha$ and $\Delta\beta$. The solution of (2)-(3) is to be calculated both at grid points, i.e., at

$$P(n, j) = (n\Delta\alpha , j\Delta\beta)$$

and at the center of rectangle grid point, i.e., at

$$P(n+\tfrac{1}{2} , j+\tfrac{1}{2}) = ((n+\tfrac{1}{2})\Delta\alpha , (j+\tfrac{1}{2})\Delta\beta)$$

where n and j are integers. We denote the approximate value of w at the grid point by $w_j^n = (n\Delta\alpha , j\Delta\beta)$.

Following the outline given above, let us consider the corresponding local Riemann problem to (2) when front is at $n\Delta\alpha$ along with the piecewise constant initial data given by

$$R_\alpha + F(R)_\beta = 0 \tag{9}$$

$$R(n\Delta\alpha, \beta) = \begin{cases} w^n_{J-1+\varepsilon} & ; \ \beta < J\Delta\beta \\ w^n_{J+\varepsilon} & ; \ \beta \geq J\Delta\beta \end{cases}$$

where

$$J = j - \tfrac{1}{2}(-1)^\varepsilon$$

$$\varepsilon = \tfrac{1}{2}(1 + sgn(\sigma_{n+1}) \cdot 1)$$

i.e. $\varepsilon = 0$ or 1 whenever σ_{n+1} is negative or non-negative respectively. The Riemann problem here is sampled at $(j+\tfrac{1}{2})\Delta\beta$ and at $(j-\tfrac{1}{2})\Delta\beta$.

When σ_{n+1} is non-negative the initial data for Riemann problem formed by using information at grid points P(n,j) and P(n,j+1) and if σ_{n+1} is negative then the initial data is constructed by using information at grid points P(n,j) and P(n,j-1). At point P(n+½, j+½) we define

$$w_{j+1/2}^{n+1/2} = R((j+\sigma_{n+1})\Delta\beta,\ (n+1/2)\Delta\alpha)$$

On each mesh interval we get a local Riemann problem. In order to assure that the waves produced by this sequence of local Riemann problems do not interact we must have

$$\frac{\Delta\beta}{\Delta\alpha} C(1+\tfrac{1}{2}m\phi) < 1. \tag{10}$$

This important requirement is known as Courant-Friedrichs-Lewy (CFL) condition. If inequality (10) holds then we can combine the solutions of the Riemann problems (9) into a single exact solution.

4 Solution of Riemann Problem

The main part of a random choice algorithm is obtaining the solutions of a sequence of local Riemann problems efficiently. The solution of a Riemann problem consists of three elementary waves, a backward shock wave or rarefaction on left, a slip line, and a forward shock or a rarefaction on right. A slip line is a discontinuous solution separating two constant states such that the angle of flows remain the same on both sides of the discontinuity line while Mach number is arbitrary. Slip lines are one family solution between the backward and forward waves, i.e., between rarefactions and shocks. To solve the Riemann problem (9) we follow Lax [6]. Let us consider the following initial data for system of equations in (9)

$$R(n\Delta\alpha, \beta) = \begin{cases} w_1 & ;\ \beta < J\Delta\beta \\ w_2 & ;\ \beta \geq J\Delta\beta \end{cases} \tag{11}$$

where subscripts 1 and 2 refer to values of w just behind of and just ahead of the discontinuity respectively. If these two values are equal then the solution of (9) is a constant state and its value is equal to the value of initial data. However, if these two values are different then the initial jump discontinuity will propagates in the form of a center expansion wave and/or a shock (i.e., jump discontinuity satisfies the entropy condition.) or a contact discontinuity. In order that solution converges to a unique weak solution of (9), it must satisfies the Rankine-Hugoniot jump condition and the Oleinik entropy condition. At the shock, let us define the values of R(α,ß) just behind of and just ahead of the shock by

$$R_1 = \lim_{\beta\to\beta^-} R(\alpha,\beta) \qquad R_2 = \lim_{\beta\to\beta^+} R(\alpha,\beta)$$

The jump conditions for system of equations (4) are given by

$$\frac{d\beta}{d\alpha} = -\frac{\theta_2-\theta_1}{A_2-A_1}$$

$$\frac{d\beta}{d\alpha} = \frac{\phi(m_2-m_1) - (\theta_2^2-\theta_1^2)}{2(A_2\theta_2 - A_1\theta_1)} \tag{12}$$

$$A_2 m_2^2 = A_1 m_1^2.$$

The entropy condition is given by

$$\frac{F(R_2)-F(R)}{R_2-R} \leq \frac{F(R_2)-F(R_1)}{R_2-R_1}$$

for any R between R_2 and R_1. The entropy satisfaction is a major concern for numerical approximation of solutions of nonlinear fluid flow problems. This simply means that the computed solution converges toward the correct physical solution as the mesh sizes of intervals along α and ß approach to zeros. The above inequality can be written as

$$E(R) = F(R_2) + \frac{d\beta}{d\alpha}(R-R_2)$$

satisfying the following inequality

$$(F(R) - F(R))\ (R_1 - R_2) \geq 0$$

where E(R) defines the chord connecting left and right limiting points across the shock. The entropy related to the first component of F is given by

$$\frac{\theta_2-\theta}{A_2-A} \geq \frac{\theta_2-\theta_1}{A_2-A_1}$$

for any A between A_1 and A_2, and θ between θ_1 and θ_2. Similar inequalities hold for other components of F.

4.1 Rarefaction Waves

Rarefaction waves are two families of solutions curves, forward and backward waves. In this section we compute the simple rarefaction waves of system of equations (9) which can be reformulated in the form

$$U_\alpha + H(U)\ U_\beta = 0$$

where H(U) = H(A, θ, m) is 3 by 3 matrix given by

$$U=\begin{pmatrix} A \\ \theta \\ m \end{pmatrix} \qquad H=\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & \frac{\phi}{2A} \\ 0 & \frac{m}{2A} & 0 \end{pmatrix}$$

The eigenvalues, μ and thier corresponding eigenvectors, e of the matrix H are

$$\mu = 0\,,\ \pm\frac{\sqrt{\phi m}}{2A}\,;\quad e=\begin{pmatrix} 1 \\ -\mu \\ -2\mu^2 A/\phi \end{pmatrix}$$

For the system of equations in (9) the simple rarefaction waves are the continuous solutions of (9) of the form

$$(13)\qquad U(\alpha,\beta)=\begin{cases} R_1 & if\ \frac{\beta}{\alpha}<\mu(R_1) \\ v(\frac{\beta}{\alpha}) & if\ \frac{\beta}{\alpha}=\mu(v) \\ R_2 & if\ \frac{\beta}{\alpha}>\mu(R_2) \end{cases}$$

where v is an integral curve of the vector field of the corresponding eigenvector connecting the two constant states such that the corresponding eigenvalue, μ is increasing between this two constant states from left to right. Since the matrix H has three distinct eigenvalues, there are three possible rarefaction waves through any given state. These rarefaction waves are the integral curves of the vector field defined by each eigenvector of matrix H, i.e., each eigenvector is tangent at each point of integral curve. Thus for the eigenvector e corresponding to the eigenvalue μ of matrix H, the integral curves are solutions the following system of equations

$$\frac{dA}{1}=\frac{d\theta}{-\mu}=\frac{dm}{-2\mu^2 A/\phi}$$

If $\mu = 0$ then the integral curves of its corresponding eigenvector, e = (1, 0, 0) are curves where θ and m are both constants. Hence a simple rarefaction wave of the form of (13) exists if the left and right values of θ and m across the shock are equal, in addition, μ must be an increasing function of θ and m from left to right across the shock. Therefore there is no A-rarefaction wave.

θ-rarefaction waves. If μ is not zero then the integral curves of its corresponding eigenvector are curves where m^2A is constant. There are two families of curves where θ is either positive or negative along each integral curve.

5 Numerical Experiments

We compared the numerical solutions using the random choice method developed here with those solutions obtained using the method of characteristics. Consider the initial condition

$$A(0,\beta)=1$$
$$m(0,\beta)=0.01$$
$$\theta(0,\beta)=\begin{cases} \frac{\pi}{12}\beta & -1<\beta<1 \\ 0 & otherwise \end{cases}$$

together with equations (2) and (4). The results obtained with both methods were very close to each other. The numerical calculations show that the convergence of the solution toward the exact solution is independent of choice of the odd number k in (7) as long as k is bounded. In addition, the method is numerically stable. All the striking physical features of system of equations (2) and (4) is observed, i.e., as the initial front propagates into the rest state the center of hump becomes flat and this flat region propagates on both directions untill the front becomes a flat surface.

6 Conclusion

The numerical solutions show that the method is stable and correctly describes the important physical feature of the solution of the model problem. The various choices of random number generators do not have any effect on the accuracy of computed solution as long as the random variable tent toward the equipartitioning of the given interval.

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An Algorithm to Estimate Parameters for a Stochastic Linear Compartmental System

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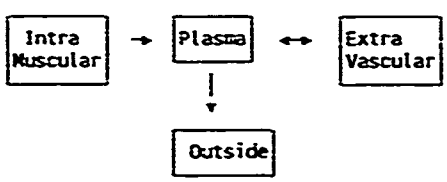
ABSTRACT. Linear compartmental systems have compartments with flows to and from the compartments. Of interest, is the estimation of the constants, θ, governing the flows. In the particular system considered, only one compartment, out of several, is observed for n cases over k time points. A stochastic model is used with a maximum likelihood approach taken to the estimation of θ. The algorithm involves iteratively using an estimate of θ to solve differential equations which describe the system, and improve on the estimate of θ by adding a constant multiple, α, of an increment $\delta\theta$. Jennrich's results are incorporated to obtain required derivatives. Due to non-zero correlations, a modification to Jennrich and Moore's results is made, involving using both the observations and their cross-products, to obtain $\delta\theta$. α is determined with Fletcher's method. A program in Turbo Pascal implements the algorithm.

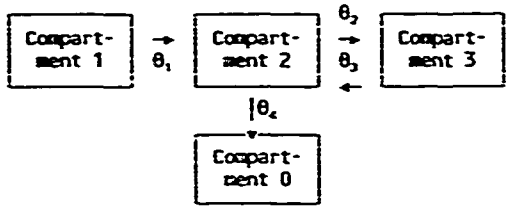
INTRODUCTION. Compartmental systems have long been a useful tool in pharmacokinetics (Wagner (1971)). The body is thought of as a series of compartments, with a drug moving between any of the compartments. For example, Gladtke et al. (1979) p. 36, suppose that the body may be represented as three compartments - plasma, muscle and extravascular. An initial muscle injection is given and the levels of the drug in,the plasma are monitored from time to time. The drugs will flow from muscle to plasma. Additionally, flow will be between the extravascular system and plasma, and from plasma to the outside, as depicted in diagram 1.

Diagram 1:



For simplicity, this paper will be restricted to a three compartmental system of this type, with compartments 1,2,3 and the outside, as compartment 0; flows have a parameter attached to them as in diagram 2, (In the traditional deterministic model, these are the rate parameters).

Diagram 2 :



It is assumed that a bolus injection is given in compartment 1 and only compartment 2 is observed, at times $t_1,t_2,\ldots,t_k$. Let θ_0 be the initial concentration in compartment 1 and C(t) be the concentration at time t.Then

$$C(t)=\begin{bmatrix}C_1(t)\\C_2(t)\\C_3(t)\end{bmatrix},\quad C(0)=\begin{bmatrix}\theta_0\\0\\0\end{bmatrix}.$$

STOCHASTIC MODEL . For the "particle model", as discussed by Purdue (1974a), it is assumed that there are N particles in the system acting independently. Transitions between compartments follow a Markov process, with the transition probability being constant. The resulting system of equations is as follows:

$$dP(t)/dt = P(t)A^T, \qquad .....(1)$$

where $P(t) = (p_{ij}(t))$ is a nonsingular 3x3 matrix with $p_{ij}(t)$, $i,j=1,2,3$, the probability of a particle transferring from compartment "i" to compartment "j" in time t and

$$A=\begin{bmatrix}-\theta_1 & 0 & 0\\ \theta_1 & -(\theta_2+\theta_4) & \theta_3\\ 0 & \theta_2 & -\theta_3\end{bmatrix}=(a_{ij}).$$

$\theta = (\theta_0\,\theta_1\,\theta_2\,\theta_3\,\theta_4)^T$ is to be estimated.

Under these assumptions it can be shown that the exact distribution of C(t), given C(0) is a multinomial (since only $C_1(0)$ is nonzero), but the distribution of $C(t_j)$, given $C(t_{j-1})$, is a convolution of multinomials. Thus, to write down the exact distribution of the concentrations in compartment 2 for $t_1,t_2,\ldots,t_k$, when k is large is impossible since it would consist of many sums whose limits are complex. Using a diffusion approximation, it has been demonstrated that the concentrations over time have a multivariate normal distribution, Lehoczky and Gaver (1977). Hence, the distribution of the concentrations in compartment 2 have a (marginal) multivariate distribution, with mean and variance-covariance matrix the same as that given by the particle model . Simpson (1988) has shown that an estimator derived from the maximum likelihood equations, using this approximate normal distribution, is still a consistent asymptotically normal estimator, if the particle model is the correct one. Thus, an algorithm was written to estimate θ using the approximate normal distribution.

Suppose that X_{ij} is the concentration in compartment 2 for person i, i=1,2,...n at time t_j, j=1,2,...k. $X_i = (X_{i1},X_{i2},\ldots,X_{ik})$ are the k observations of ith case. $X_1,X_2,\ldots,X_n$ are independently and identically distributed as a normal variable with mean and variance which are functions of the probability matrix P. By considering a vector comprised of the sufficient statistics of the covariance of X, it can be seen that a normally distributed random variable is a linear exponential and so the algorithm of Jennrich and Moore (1975) ,hence referred to as JMA, can be used to find the approximate maximum likelihood estimator . We take the k_1x1 vector Y, where $k_1 = k(k+3)/2$ and

$$Y=\frac{1}{n}\Big[\sum_{r=1}^{n}X_{r1},\sum_{r=1}^{n}X_{r2},\ldots\ldots,\sum_{r=1}^{n}X_{rk},\sum_{r=1}^{n}X_{r1}^2,\sum_{r=1}^{n}X_{r1}X_{r2},\ldots\sum_{r=1}^{n}X_{r1}X_{rk},\sum_{r=1}^{n}X_{r2}^2,\ldots\ldots\ldots,\sum_{r=1}^{n}X_{r2}X_{rk},\ldots\ldots\ldots\ldots\ldots,\sum_{r=1}^{n}X_{rk-1}^2,\sum_{r=1}^{n}X_{rk-1}X_{rk},\sum_{r=1}^{n}X^2{}_{rk}\Big]$$

Using properties of normality,Y has a mean, $\mu(\theta)$, and variance-covariance matrix, $\Sigma(\theta)$, which is a function of the mean and variance-covariance matrix of X, and therefore of P, also.

THE ALGORITHM. Suppose that the k_1x5 matrix of partial derivatives with respect to θ_i, i=0,1,..,4 is denoted by $d\mu/d\theta$. According to the JMA, for a given θ, replace θ by $\theta+\alpha\delta\theta$,where

$$\delta\theta=\left[\left(\frac{d\mu}{d\theta}\right)^T\Sigma^{-1}\frac{d\mu}{d\theta}\right]^{-1}\left(\frac{d\mu}{d\theta}\right)^T\Sigma^{-1}(y-\mu)$$

This requires that
(1) P(.) and its derivatives with respect to θ be obtained
(2) $\delta\theta$ be calculated.
(3) An appropriate α be found.

(1) P(.) and its derivatives:
For this compartmental system, P(.) and its derivatives can be calculated analytically. However, to maintain generality for the program, it was decided to obtain P(.) and its derivatives by applying the method developed by Allen (1987) to columns of P(.).

The steps, for each column of P, are as follows:
(i) Find R so that
- $R^TAR = T$, a triangular matrix.
- $R^TR = I$, the identity matrix

(ii) Using R, obtain a triangular system of equations; so, a backward solving technique can be used, with the initial condition $P(0) = I$ satisfied.

For any θ_a, a=1,2,3,4, the equation (1) becomes

$$\frac{dV_a}{dt}(t)=AV_a(t)+R^T\frac{\partial A}{\partial\theta_a}R\,R^TX(t),$$
$$RV_a(t)=\frac{\partial X(t)}{\partial\theta_a}$$

and Allen's method can be used again to solve for $V_a(t)$, with $V_a(0) = 0$, as the initial condition

(2) Calculation of $\delta\theta$:
Using Wilkinson's algorithms, Wilkinson (1971), a Cholesky decomposition is used to find $\Sigma^{1/2}$, where $\Sigma^{1/2}(\Sigma^{1/2})^T=\Sigma$. Using this, the following equation is solved to obtain $\delta\Theta$:

$$\mu_1=\Sigma^{1/2}\frac{d\mu}{d\theta}$$
$$y_1=\Sigma^{1/2}(y-\mu)$$
$$\mu_1^T\mu_1\delta\theta=\mu_1^Ty_1$$

(3) An α:
Fletcher's descent method, Fletcher (p.26, 1980) is used to find α. It uses the first derivatives only. Assuming uniform continuity conditions, it will achieve, at least, a local optimum if an optimum exists and if the starting value is close enough.

SUMMARY. A stochastic approach rather than the traditional deterministic model approach is taken to a particular compartmental model, where only one compartment is observed. An algorithm is developed which uses the JMA to obtain maximum likelihood estimates from a diffusion approximation. The program is written in Turbo Pascal and can be generalised:
(i) to other linear compartmental systems,
(ii) for θ to be functions of time,
Work is being done:
(iii) to incorporate measurement error in the model
(iv) to include people variation

An important step for its general use would be to incorporate this program in a general pharmacokinetic program so that, in a user friendly environment, its estimates could be easily compared to those obtained from other methods.

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